A LINAN

The structure of diffusion flames

1. INTRODUCTION

These notes are devoted to the analysis of reacting flows in systems where the reactants are initially unpremixed. We shall deal here with the combustion reactions, encountered very often in applications, which take place in the gas phase, between a fuel and an oxidizer, (typically the oxygen of the air). The combustion reactions are exothermic, so that we shall see large temperature differences in the flow field, and the reaction rates are very sensitively dependent on temperature. Then in regions of the flow field where the temperature is low the reactants will mix without chemical reactions, while in regions of high temperature the flow will be in chemical equilibrium. When the reaction can be modelled by an overall irreversible reaction between the fuel and the oxygen, the chemical equilibrium condition implies that one of the reactants has locally zero concentration, because it has been previously completely consumed by the chemical reaction. The chemical reaction has taken place in thin reaction layers in the form of rich or lean premixed flames, when they separate regions of frozen flow from regions of equilibrium flow, or diffusion flames, when they separate a region without fuel from a region without oxidizer.

Diffusion flames are formed in large variety of natural and industrial systems. We find diffusion flames in fires, in industrial furnaces, in Jet and Diesel engine combustion chambers, and also in the combustion chamber of Rocket engines.

Very often the fuel is initially in solid or liquid form, so that, for example, the solid must gasify before mixing and chemical reaction with the oxygen may take place in the gas phase. The liquid fuels are injected in the combustion chamber in the form of jets that break, or atomize, to form a spray of small droplets that vaporize to generate the fuel vapors that mix and react with the ambient air.

In the following, we are forced to restrict our discussion to some theoretical aspects of the analysis of combustion in unpremixed systems; so that we will limit our considerations to gaseous systems undergoing chemical reactions that can be modelled by an overall irreversible Arrhemius reaction.

For a more complete description of the combustion processes, the reader may consult the other Lecture Notes in this Course, and, for example the books by Williams (1985) and Zeldovich et al. (1984), the chapter on Combustion in the book of Frank-Kamenetskii (1969) and also the book by Buckmaster and Ludford (1981) on the asymptotic analysis of Combustion.

In the following we shall begin in Section II with the formulation of the conservations equations, and a consideration of the characteristic scales and parameters introduced by the initial and boundary conditions.

Section III will be devoted to a description of the limiting case of very fast reactions, when they take place in thin layers, or reaction sheets at a diffusion controlled rate.

In Section IV we will introduce the large activation energy analysis of diffusion flames, where we shall encounter the triple flame structure mentioned earlier in the Introduction. Section V will be devoted to the analysis of diffusion flames in strained mixing layers where we encounter the concepts of ignition and extinction of diffusion flames.

2. FORMULATION

We shall give below the conservation equations that describe the process of gas phase mixing and chemical reaction between a fuel and an oxidizer, for example the oxygen of the air. The reaction will be modelled by an overall reaction of the form

$$F + \nu_0 0_2 \rightarrow (1 + \nu_0)P + (q) \tag{1}$$

where a mass ν_0 of Oxygen is consumed per unit mass of fuel to yield a mass $(1 + \nu_0)$ of products and a thermal energy q.

Let $\vec{v}$, ρ, p, T be the velocity, density, pressure and temperature of the fluid; and let Y_F, Y_0 and Y_p be the mass fractions of the fuel, oxygen and products (i.e. the ratio of their densities to the fluid density). These variables are functions of the time t and spatial coordinate $\vec{x}$, given by the following system of conservation equations, see Williams (1985),

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{v}) = 0 \tag{2}$$

$$\frac{\partial}{\partial t}(p\vec{v}) + \nabla \cdot (\rho \vec{v}\vec{v}) = \rho \vec{g} - \nabla p + \nabla \cdot \tau' \tag{3}$$

$$\frac{\partial}{\partial t}(\rho Y_\alpha) + \nabla \cdot (\rho \vec{v} Y_\alpha) = \nabla \cdot (\rho D_\alpha \nabla Y_\alpha) + w_\alpha \tag{4}$$

$$\frac{\partial}{\partial t}(\rho c_p T) + \nabla \cdot (\rho \vec{v} c_p T) = \nabla \cdot (k \nabla T) - q w_F \tag{5}$$

together with the equation of state

$$p = \rho T R / M \tag{6}$$

where R is the universal gas constant and M is the mean molecular mass that we shall, for simplicity consider constant. The specific heat at constant pressure c_p, appearing in Eq. (5) will also be considered to be constant.

The energy conservation Eq. (5) has been written in the simplified form appropriate for the analysis of combustion in flows with low Mach numbers in an open atmosphere. In these flows the spatial variations in pressure, determined by the momentum Eq. (3) which includes the gravity force $\vec{g}$, are small compared with the pressure itself, and these may be neglected in Eq. (6), where p may be approximated by a constant typical value p_a of the pressure in the flow field. In Eqs. (3)-(5) the viscous stress tensor τ' and the diffusion and heat conduction fluxes are given by the well known laws of Navier-Poisson, Fick and

Fourier in terms of the gradients of velocity, mass fractions and temperature. D_α is the diffusivity of the species α, and D_T is the thermal diffusivity. The ratio $D_T/D_\alpha = L_\alpha$, the Lewis number of the species α, will be assumed to be constant, while ρD_T will be considered a known function of T. Eq. (4) is applicable to any species in the fluid mixture. The reaction term $W_\alpha = 0$ for any inert species (like N_2), and

$$W_0/\nu_0 = -W_p/(1+\nu_0) = W_F \tag{7}$$

where we shall use for W_F the Arrhenius overall expression

$$W_F = -\rho B e^{-E/RT} Y_0 Y_F \tag{8}$$

where B is a frequency factor, and E the activation energy of the reaction.

With this form, Eq. (8), of the rate expression, and the assumption that the mean molecular mass M is constant, we only need two species conservation equations (4), for the fuel and oxygen mass fractions Y_F and Y_0 for the description of the flow field.

When solving the system of conservation equations (2)-(8) we must add as initial conditions the values of the mass fractions of the species, together with the initial temperature and velocity distributions. We must also give the temperature and velocity of the fluid at the boundary, together with the condition that the derivatives of the mass fractions of the species normal to the boundary is zero at a non-reacting boundary.

We shall not attempt to write these boundary conditions in more detailed form, but we must indicate that they provide the characteristic times, velocities and lengths of the flow.

As an example, we consider a jet of fuel coming out into ambient air, through an injector of radius a. We must specify the temperature T_0, fuel mass fraction Y_{FO} and velocity distribution upstream in the injector; this velocity distribution is characterized by a mean velocity U. The air may be stagnant far from the injector, with a temperature T_a (that for simplicity in the presentation we shall consider equal to T_0) and an oxygen mass fraction Y_{00}. The product and oxygen concentration upstream in the fuel feed stream will be assumed to be zero, while the product and fuel concentration in the ambient air will also be zero. The derivatives of the mass fractions normal to the injector wall are zero, while the temperature of the fluid at the interface with the injector must be equal to that of the injector; in the extreme case where the injector walls are highly conducting this temperature will be T_0; while in the opposite case we will consider the wall to be adiabatic and the normal derivative of T at the wall surface will be zero. If the injector velocity, for example, changes with time, a characteristic time is introduced by the time t_0 required to change the velocity by a factor of order 1.

The boundary conditions thus introduce characteristic values U, a and t_0 for the velocity, length and time. These can be used for a naive estimate of the order of magnitude of the different terms in the conservation equations. Thus, we give below, the order of the terms in the conservation equation for the fuel mass fraction

$$\frac{\partial Y_F}{\partial t} + \overline{v} \cdot \nabla Y_F - \rho^{-1} \nabla \cdot (\rho D_F \nabla Y_F) = -Be^{-E/RT} Y_0 Y_F \tag{9}$$

$$t_0^{-1} \qquad U/a \qquad\qquad D_F/a^2 \qquad\qquad t_{ch}^{-1}$$

if we consider Y_{FO} and Y_{00} to be of order unity, and consider that, at a typical point of the flow field at a distance of order a from the injector, Y_F and Y_0 are of order unity and undergo changes of order unity in times of order t_0, and when, at a given time, we move a distance of order a. The characteristic chemical time t_{ch} is of the order of the inverse of the reaction constant $B\exp(-E/RT)$.

When the times t_0, a^2/D_F and t_{ch} that characterize the terms representing the local accumulation, the diffusion and the chemical reaction are compared with the residence time a/U that measures the convective term we obtain the parameters

$St = a/Ut_0 =$ Strouhal number;

$Pe = aU/D_F =$ Peclet number;

$Da = a/Ut_{ch} =$ Damköhler number.

These parameters measure the relative importance of the different terms in the conservation equation for the fuel. In gases the Lewis numbers and the Prandtl number, ratio of the kinematic viscosity ν to the thermal diffusivity, are of order unity, so that the Peclet and Reynolds numbers are of the same order. Thus the same parameters measure, also, the relative importance of the different terms in the other conservation equations.

If the Strouhal number is small compared with unity we introduce the quasi-steady approximation: neglecting the unsteady, accumulation terms, in the equations.

If the Reynolds or Peclet number were small compared with unity, we could neglect the convective term relative to the diffusive term; this is the case when analysing the vaporization and combustion of "small" fuel droplets moving at "small" relative velocities in air.

In many applications in Combustion the characteristic values of the Reynolds numbers are large compared with unity. In this case the diffusion term can be neglected in most of the flow field; then mixing of the reactants is confined to thin mixing layers, of thickness δ_m such that

$$\delta_m^2/D_F = a/U \ . \tag{10}$$

The characteristic diffusion time across the layers is of the order of the residence time. The chemical reaction is obviously confined to these layers.

The mixing layers at high Reynolds numbers are also, typically, thin vorticity layers, introduced in the analysis of fluid flows by Helmholtz in 1868 and shown by Kelvin in 1871 to be unstable to small disturbances; see Drazin and Reid (1981). Due to the Helmholtz-Kelvin instabilities, the flow in the mixing layers becomes turbulent: the vorticity first concentrates in discrete vortices that grow in size by pairing (in a non periodic way), and are also subject to three-dimensional instabilities that produce vortices of smaller and smaller scale.

The mixing layers are strongly corrugated by the unsteady, three-dimensional, turbulent flow, so that mixing is very much enhanced by the turbulence. For this reason, in order to reduce the size of the combustion chambers, or increase their output, these are designed for the flow to be turbulent. For the description of the fluctuating temperature, velocity and concentration fields we can use the conservation equations written above, with the terms representing the local accumulation, convection and diffusion of the same order in the regions where molecular mixing and reaction take place; the characteristic times associated with accumulation, convective transport and diffusion are of the same order t_λ for the eddies of size λ, of typical velocity V_λ given according to the Kolmogorov by the relations

$$V_\lambda^3/\lambda = V^3/l \ , \ t_\lambda = \lambda/V_\lambda \tag{11}$$

in terms of the eddy size λ and characteristic velocity V and size l of the large eddies. These relations can be used for eddy sizes smaller than l and larger than the Kolmogorov eddy size l_k, given by (11) and the condition $V_k l_k/\nu = 1$. For the flow with velocity U coming out of an injector of size a, $l \sim a$ and $V \sim U$.

The importance of the reaction term relative to the convective transport term (the most of important of the transport terms in high Reynolds number flows) is measured by the Damköhler number:

$$D_a = aU^{-1}Be^{-E/RT} \tag{12}$$

whose value may change across the flow field due to the changes in the Arrhenius exponential with temperature. In a turbulent flow the residence time a/U, should be replaced by $(\lambda/a)^{2/3}a/U$, when measuring the importance of the reaction term in the thin mixing layers surrounding an eddy of size λ.

When the Damköhler number is everywhere in the flow field $Da \ll 1$, the reactants can not coexist in the flow field. If the order of magnitude of the terms in the left hand side of Eq. (9) is U/a and $Be^{-E/RT}$ is $O(t_{ch}^{-1})$, then we may conclude that

$$Y_F Y_0 = 0(t_{ch}U/a) = 0(D_a^{-1}) \ .$$

This implies, in the limit $D_a \to \infty$, that Eq. (9) simplifies to

$$Y_F = 0 \quad \text{or} \quad Y_0 = 0 \ . \tag{13}$$

The reactants can not coexist; the flowfield is divided in two domains Ω_F and Ω_0 separated by a reaction sheet Σ_f. In the fuel domain Ω_F, $Y_0 = 0$ the oxygen concentration is zero. In the oxygen domain Ω_0, $Y_F = 0$. Both reactants have zero concentration at the surface Σ_f, where the chemical reaction takes place.

3. THE BURKE-SCHUMANN ANALYSIS OF DIFFUSION FLAMES

In 1928 Burke and Schumann showed how the structure of diffusion flames could be described in the limiting case of very fast reactions. The Burke-Schumann (B-S) description corresponds to the limit $D_a \to \infty$, when the reactants can not coexist.

The temperature and concentration profiles are shown schematically in Fig. 1 for a given cross-section AA'. The profiles show the temperature and concentration distributions as continuous but with discontinuous derivatives at the flame sheet Σ_f. The discontinuities are associated with a Dirac delta form of the reaction terms in the conservation equations

$$\frac{\partial Y_F}{\partial t} + \vec{v} \cdot \nabla Y_F - (\rho L_F)^{-1} \nabla \cdot (\rho (D_T \nabla Y_F) = W_F/\rho \tag{14}$$

$$\frac{\partial Y_0}{\partial t} + \vec{v} \cdot \nabla Y_0 - (\rho L_0)^{-1} \nabla \cdot (\rho D_T \nabla Y_0) = \nu_0 W_F/\rho \tag{15}$$

$$\frac{\partial T}{\partial t} + \vec{v} \cdot \nabla T - \rho^{-1} \nabla \cdot (\rho D_T \nabla T) = -(q/c_p) W_F/\rho \tag{16}$$

for the concentrations and temperature.

The Dirac delta character of the non-dimensional reaction term $-\frac{a}{U} W_F/\rho = (a/U) B e^{-E/RT} Y_F Y_0 = D_a Y_F Y_0$ is associated with the limit $Da \to \infty$, which leads to a zero value of W_F outside the flame sheet and an infinite value of W_F at the flame sheet.

From the asymptotic structure of the solution, represented in Fig. 1, we can anticipate that in the thin reaction zone the large reaction terms are balanced by the diffusion terms normal to the flame sheet. That is

$$-\frac{1}{\rho}\frac{\partial}{\partial n}\{\rho D_T \frac{\partial}{\partial n}\left(\frac{Y_E}{L_F}\right)\} = -B e^{-E/RT} Y_F Y_0 \tag{17}$$

$$-\frac{1}{\rho}\frac{\partial}{\partial n}\{\rho D_T \frac{\partial}{\partial n}\left(\frac{Y_0}{L_0}\right)\} = -\nu_0 B e^{-E/RT} Y_F Y_0 \tag{18}$$

$$-\frac{1}{\rho}\frac{\partial}{\partial n}\{\rho D_T \frac{\partial}{\partial n}(T)\} = \frac{q}{c_p} B e^{-E/RT} Y_F Y_0 \tag{19}$$

where n is the outer normal distance to the flame sheet. The reaction terms can be eliminated from these equations, and then integrated across the flame sheet to yield

$$-\rho D_T \frac{\partial}{\partial n}\left(\frac{Y_F}{L_F} - \frac{Y_0}{\nu_0 L_0}\right) = m''_F = m''_0/\nu_0 \tag{20}$$

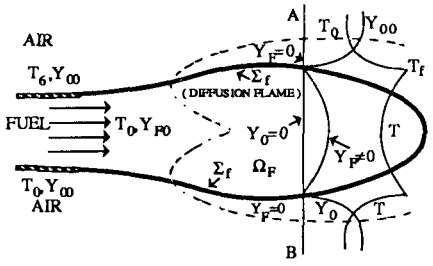

Figure 1. The temperature and concentration profiles of diffusion flames in the Burke-Schumann limit.

$$\left(\rho D_T \frac{\partial T}{\partial n}\right)_{-\infty} - \left(\rho D_T \frac{\partial T}{\partial n}\right)_{+\infty} = q m_F''/c_p \tag{21}$$

when we take into account that $Y_F = 0$ at $n \to \infty$ and $Y_0 = 0$ at $n \to -\infty$.

In these relations m_F'', m_0'' and $q m_F''$ are, respectively, the rate of mass consumption of fuel and oxygen, and the rate of heat release per unit flame surface and time. Thus, the reactants reach the flame sheet, from opposite sides, by diffusion at stoichiometric proportions; the heat released by the reaction, $q m_F''$ per unit flame surface and time, is conducted away from the flame sheet.

Thus for the Burke-Schumann description of the diffusion flame, we should solve Eqs. (14) and (16), with $W_F = 0$ and $Y_0 = 0$ in Ω_F (the fuel side of the flow field), and Eqs. (15) and (16), with $W_F = 0$ and $Y_F = 0$ in Ω_0 (the oxygen side of the flow field). The flame sheet Σ_f must be determined as a free boundary problem by requiring that Y_F, Y_0 and T are continuous at the flame sheet and satisfy there the jump conditions given by Eqs. (20) and (21). Burke and Schumann (1928) indicated how this problem could be solved when the Lewis numbers of the fuel and oxygen are equal to unity (the equidiffusional approximation): in this case the linear combinations $(Y_F - Y_0/\nu_0)$ and $Y_F + c_p T/q$ diffuse like passive scalars. These so called, Schvab-Zeldovich, coupling functions have been widely used with the equidiffusional approximation. See Williams (1985).

We generalize here this approach to the general case of non-unity Lewis numbers. See Liñán (1989) for the details of the analysis.

Let us define first the generalized mixture fraction variable

$$Z = (S\hat{Y}_F + 1 - \hat{Y}_0)/(S+1) \tag{22}$$

where

$$\hat{Y}_F = Y_F/Y_{FO}\ ,\ \hat{Y}_0 = Y_0/Y_{00} \qquad \text{and} \qquad S = \nu_0 Y_{FO} L_0/Y_{00} L_F \tag{23}$$

is a generalized air fuel stoichiometric ratio. The mixture fraction variable Z is a normalized coupling function, $Y_F/L_F + (Y_{00} - Y_0)/\nu_0 L_0$, which according to Eq. (20) diffuses without reaction across the flame sheet. The normalization, by division by its value on the fuel feed stream, insures that $Z = 1$ in the fuel feed stream, and $Z = 0$ in the ambient air.

A conservation equation for Z can be obtained by substracting from Eq. (14), Eq. (15) divided by ν_0. We thus obtain the equation

$$L_e(Z)\rho\left(\frac{\partial Z}{\partial t} + \vec{v}\cdot\nabla Z\right) - \nabla\cdot(\rho D_T \nabla Z) = 0 \tag{24}$$

if we take into account that, according to the (B-S) equilibrium conditions, Eq. (13),

$$Y_0 = 0 \quad \text{for} \quad Z > Z_s \quad \text{and} \quad Y_F = 0 \quad \text{for} \quad Z < Z_s \tag{25}$$

with, Z_s, the stoichiometric value of the mixture fraction, defined by

$$Z_s = 1/(s+1) = (1 + \nu_0 Y_{FO} L_0/Y_{00} L_F)^{-1} \tag{26}$$

and $L_e(Z)$, an effective Lewis number, defined by

$$L_e = L_F \quad \text{for} \quad Z > Z_s \quad \text{and} \quad L_e = L_0 \quad \text{for} \quad Z < Z_s\,. \tag{27}$$

Eq. (24) is a non-linear conservation equation for the modified mixture fraction variable Z, which, together with Eq. (25) may used to replace Eqs. (14) and (15). In the particular case when the Lewis numbers are equal to unity, Z reduces to the widely used form of the mixture fraction variable Z, described by the linear conservation equation (24) with $L_F = L_0 = 1$.

The flame surface is given by the level surface

$$Z(\vec{x}, t) = Z_s \tag{28}$$

of the mixture fraction variable.

A similar conservation equation free from the reaction term can be obtained from Eqs. (14)-(16), to replace Eq. (16) when analysing the structure of diffusion flames in the (B-S) limit of infinite Damköhler numbers. Thus if we add Eq. (14) to Eq. (15) multiplied by S/ν_0 to Eq. (16) multiplied by $(1+S)c_p/q$, we obtain, if Eq. (25) is taken into account, the following conservation equation

$$N(Z)\rho\left(\frac{\partial Z}{\partial t} + \vec{v}\cdot\nabla Z\right) + \rho\left(\frac{\partial H}{\partial t} + \vec{v}\cdot\nabla H\right) - \nabla\cdot(\rho D_T \nabla H) \tag{29}$$

for the excess enthalpy H, defined by

$$H = \hat{Y}_F + \hat{Y}_0 - 1 + (1+S)L_F c_p(T - T_0)/qY_{FO} \tag{30}$$

where

$$N(Z) = (L_F - 1)(S + 1)/S \quad \text{if} \quad Z > Z_s \tag{31a}$$

$$N(Z) = (1 - L_0)S + 1 \quad \text{if} \quad Z < Z_s \, . \tag{31b}$$

The excess enthalpy function H is equal to zero in the fuel feed stream, and also in the ambient unperturbed air side of the diffusion flame.

The temperature and concentrations will then be given in terms of Z and H by the relations.

$$H + (1 + 1/S)(1 - Z) = (1 + S)L_F c_p(T - T_0)/qY_{FO} \tag{32a}$$

when

$$\hat{Y}_0 = 0 \, , \; S\hat{Y}_F = (S + 1)Z - 1 \geq 0$$

and

$$H + (1 + S)Z = (1 + S)L_F c_p(T - T_0)/qY_{FO} \tag{32b}$$

when

$$\hat{Y}_F = 0 \, , \quad \hat{Y}_0 = 1 - (1 + S)Z \geq 0 \, .$$

For unity Lewis numbers, $N = 0$. If, in addition, the walls of the injector are adiabatic the solution of Eq. (29) gives $H \equiv 0$, and the flame sheet temperature T_f takes the adiabatic flame temperature value T_e,

$$T_e = T_0 + qY_{FO}/c_p(1 + S) \, . \tag{33}$$

For other values of the Lewis numbers, the flame sheet temperature takes the value

$$T_f = T_0 + (H_f + 1)qY_{FO}/c_p L_F(1 + S) \tag{34}$$

where H_f, the value of H at $Z = Z_s$, is no-zero due to the so called preferential diffusion effects.

In summary, when describing the diffusion flame structure in the (B-S) limit of infinite Damköhler numbers, the conservation equations (14)-(16), which include, in their right hand sides, Dirac delta functions of initially unknown strength placed at an unknown flame surface, may be replaced by the equilibrium conditions (32) and the non-linear transport equations (24) and (29) for Z and H. These equations can be written in conservation form

$$\frac{\partial}{\partial t}(\rho G) + \nabla \cdot (\rho \vec{v} G) - \nabla \cdot (\rho D_T \nabla Z) = 0 \tag{35}$$

$$\frac{\partial}{\partial t}\{\rho(K + H)\} + \nabla \cdot \{\rho \vec{v}(K + H)\} - \nabla \cdot (\rho D_T \nabla H) = 0 \tag{36}$$

in terms of the functions $G(Z)$ and $K(Z)$, defined by

$$G = (Z - Z_s)L_e(Z) \quad \text{and} \quad K = (Z - Z_s)N(Z) \, . \tag{37}$$

This description of the diffusion controlled combustion process will be particularly useful in the modelling of turbulent combustion flows, or in their direct numerical simulation.

Finally, we shall indicate that if we are interested in the description of the reaction zone structure for large but finite values of the Damköhler number, we should notice that the reaction is confined to a thin layer placed along the flame sheet surface, given by $Z = Z_s$ with the (B-S) description. Outside the reaction layer the temperature and concentrations are well described by the (B-S) solution.

In the reaction layer, as first shown by Liñán (1961) and later by Fendell (1965), the conservation equations reduce to Eqs. (17) and (19), representing a reactive-diffusive balance. These equations can be additionally simplified because the differences of T from T_f are so small at large Damköhler numbers that the Arrhenius factor can be replaced by $\exp(-E/RT_f)$, and in addition, ρ and D_T by their (B-S) flame sheet values ρ_f and D_{Tf}. Then the conservation equations take the form

$$\frac{\partial^2 Y_F}{\partial n^2} = L_F D_{Tf}^{-1} B e^{-E/RT_f} Y_F Y_O \tag{38}$$

$$\frac{\partial}{\partial n}(Y_O/\nu_O L_O - Y_F/L_F) = m''_F/\rho_f D_{Tf} \tag{39}$$

$$\frac{\partial^2 H}{\partial n^2} = 0 \tag{40}$$

where Eq. (39) and (40), with H defined by Eq. (30), are combinations of Eqs. (17) and (19). Eqs. (38)-(40) must be solved with the boundary conditions obtained by matching with the outer $(B - S)$ solutions.

Then

$$H = H_f + nH_{nf} \tag{41}$$

where $H_{nf} = \partial H/\partial n$, evaluated at the flame sheet $Z = Z_s$ using the $(B - S)$ solution.

Similarly, Eq. (39) can be integrated to yield

$$Y_O/\nu_O L_O - Y_F/L_F = nm''_F/\rho_f D_{Tf} \tag{42}$$

where

$$L_F m''_F/\rho_f D_{Tf} = -Y_{FO}(1 + 1/S)Z_{nf} \tag{43}$$

and

$$Z_{nf} = \partial Z/\partial n \quad \text{at} \quad Z = Z_s \, .$$

Eq. (38) can be used with Eq. (42), and the boundary conditions

$$Y_F = 0 \quad \text{at} \quad n \to \infty \, , \; Y_O = 0 \quad \text{at} \quad n \to -\infty \tag{44}$$

to calculate $Y_F(n)$ and $Y_O(n)$; the temperature will then be given by Eq. (41).

The equation for Y_F takes the normalized form

$$d^2y/d\eta^2 = y(y+\eta) \tag{45}$$

and the boundary conditions

$$y = 0 \quad \text{at} \quad \eta \to \infty \ , \ y + \eta = 0 \quad \text{at} \quad \eta \to -\infty \tag{46}$$

with the appropriate scaling of the variables Y_F and n. The resulting value of Y_F in the reaction zone is of order

$$Y_{Fr} \sim D_a^{-1/3} = \{Bd^2 D_{T_f}^{-1} \exp(-E/RT_f)\}^{-1/3} \tag{47}$$

where $1/d$ is the $(B-S)$ value, at the flame sheet, of the gradient of the fuel mass fraction, given by the right hand side of Eq. (43).

The corresponding changes, from T_f, of the temperature in the reaction zone are of order $(T_e - T_0)D_a^{-1/3}$. When these changes become, for more moderate values of the Damköhler number, of order RT_f^2/E, the Arrhenius factor can not be approximated by a constant factor, and we encounter the extinction regime described by Liñán (1974).

Let us analyse, as an example, the combustion of a spherical fuel pocket in air. For simplicity in the presentation, we shall carry out the analysis using the thermal-diffusive approximation; in this approximation the velocities induced by the thermal expansion are neglected, or equivalently the density is considered constant. In addition, we shall consider the case in which the Lewis numbers are equal to 1.

For the initial conditions, at $t = 0$, we take

$$T = T_0 \ , \ Y_F = Y_{FO} \ , \ Y_0 = 0 \quad \text{at} \quad r < a \tag{48a}$$

$$T = T_0 \ , \ Y_F = 0 \ , \ Y_0 = Y_{00} \quad \text{at} \quad r > a \ . \tag{48b}$$

Then in the $(B-S)$ limit of infinite Damköhler numbers, the temperature and concentration distributions are given by Eqs. (32) with $H \equiv 0$ and Z given by the equation

$$\frac{\partial Z}{\partial \tau} - \frac{1}{x^2}\frac{\partial}{\partial x}\left(x^2 \frac{\partial Z}{\partial x}\right) = 0 \tag{49}$$

where $x = r/a$ and $\tau = tD_F/a^2$.

This equation has to be solved, for $\tau = 0$, with the initial conditions

$$Z = 1 \quad \text{for} \quad x < 1 \ , \quad Z = 0 \quad \text{for} \quad x > 1 \ . \tag{50}$$

The solution is

$$Z = \frac{1}{2} erfc\left(\frac{1+x}{2\sqrt{\tau}}\right) + \frac{1}{2} erfc\left(\frac{1-x}{2\sqrt{\tau}}\right) - \frac{\sqrt{\tau}}{x\sqrt{\pi}}\left(e^{-\frac{(1-x)^2}{4\tau}} - e^{-\frac{(1+x)^2}{4\tau}}\right) \ . \tag{51}$$

The flame sheet is given by $Z(x,\tau) = Z_s$. It disappears at $\tau = \tau_f$ given by

$$Z_s = erfc(1/2\sqrt{\tau_f}) - (\pi\tau_f)^{-1/2}\exp(-1/4\tau_f) \ . \tag{52}$$

4. LARGE ACTIVATION ENERGY ASYMPTOTICS

We shall indicate in this Section how the large activation energy, $E/RT_0 \gg 1$, of the exothermic, $q/c_pT_0 \sim 1$, combustion reactions determines the structure of diffusion flames.

Due to the exothermicity of the combustion reaction we will find temperatures in the flow field ranging from T_0 to T_e. (In this discussion we consider for simplicity the case $L_F = L_0 = 1$). Due to the large activation energies, the characteristic reaction times t_{cho} and t_{che} at the initial and flame temperature satisfy the inequality

$$t_{cho} = B^{-1}e^{E/RT_0} \gg t_{che} = B^{-1}e^{E/RT_e} \ . \tag{53}$$

Then, the Damköhler number

$$D_a = au^{-1}Be^{-E/RT} \tag{54}$$

changes very much across the flowfield.

Let us define a cross-over temperature T_c given by

$$au^{-1}Be^{-E/RT_c} = 1 \ . \tag{55}$$

Then if $T_c < T_0$, the Damköhler number will be $D_a \gg 1$, everywhere in the flow field, and the combustion process will be diffusion-controlled well described by the Burke-Shumann limit. When $T_c > T_e$, the chemical reaction will be frozen everywhere.

In the important case $T_0 < T_c < T_e$ we will find equilibrium flow with either $Y_F = 0$ or $Y_0 = 0$ in regions of temperature higher than T_c, while the reactions will be frozen in regions where $T < T_c$.

The regions of equilibrium flow are separated from the regions of frozen mixing by thin reaction sheets of the premixed flame type, where one of the reactants is completely consumed, with only partial consumption of the other. The fuel free region is separated from the oxygen free region by a diffusion flame sheet. See Fig. 2.

In order to understand why this is so, let us write the conservation equation (9) for the fuel in the form

$$-(a/u)\left\{\frac{\partial Y_F}{\partial t} + \overline{v}\cdot\nabla Y_F - \rho^{-1}\nabla\cdot(\rho D_F\nabla Y_F)\right\} = e^{\frac{E}{RT_c}\frac{T-T_c}{T}}Y_FY_0 \ . \tag{56}$$

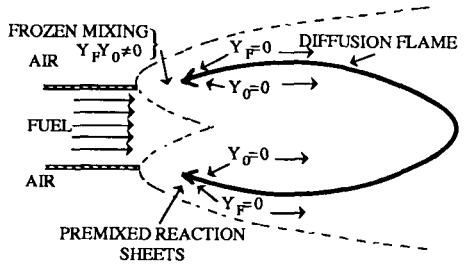

Figure 2. The triple flame structure of diffusion flames.

While we may expect each of the transport terms in the left hand side of the equation to be 0(1), the reaction term in the right hand side will be infinitely small for $T < T_c$ if $E/RT_c \to \infty$, leading to frozen flow. For $T > T_c$, the Arrhenius factor $\exp\{(E/RT_c)(T-T_c)/T\}$ will become infinitely large when $E/RT_c \to \infty$, so that the factor $Y_F Y_O$ must be infinitely small because the two members in Eq. (56) must balance.

The reaction term in the limit, $E/RT_c \to \infty$, of infinite activation energies becomes a Dirac delta function placed at a reaction sheet, where $T = T_c$; the reaction is balanced at the premixed flame sheet by the term representing diffusion normal to the sheet. At the flame sheet the temperature and concentrations are continuous, with either $Y_F = 0$ or $Y_O = 0$ at the flame sheet and also in the equilibrium side. There are, however, jumps of the temperature and concentration gradients related by the stoichiometric coefficients of the reaction (1).

The reaction term is also of the Dirac delta type in the diffusion flame sheet that separates the equilibrium regions. Along the diffusion flame sheet the temperature rises from T_c, the value at its leading edge where it meets the premixed flames, to T_e well downstream, where the cooling effect of the injector walls is no longer felt, and thereby $H_f = 0$. If the injector walls are good conductors of heat their temperature will be close to T_0; if heat from the triple flame system reaches the injector walls by heat conduction H will be negative in the triple flame region, so that the flame sheet temperature may be $T_c < T_e$ at its leading edge. See Liñán (1988).

Upstream heat conduction is essential for the diffusion flame to be anchored close to the injector lips, with a leading edge temperature $T_c < T_e$. The triple flame region, in flows with large Reynolds numbers, lies in the Navier-Stokes region at the core of the triple deck region formed at the lip of the injector; see Daniels (1977). It turns out that the characteristic residence time in this flame attachement region, to be used in the evaluation means of Eq. (55), of the flame temperature T_c, is precisely a/U, if the fuel flow velocity profile at the injector exit is parabolic. Otherwise, the injector radius a should be replaced in Eq. (55) by the fuel flow boundary layer thickness at the injector exit.

Notice that, according to Eq. (55), T_c will grow with the flow velocity U. When this velocity grows to a value U_L such that

$$aU^{-1}\exp(-E/RT) = 1 \ , \tag{57}$$

the triple flame will lift-off from the injector lip. It will move downstream to a lift-off height where, in a rough way of speaking, its upstream velocity equals the local flow velocity. The determination of the lift-off height is difficult if the flow is turbulent, when the triple flame will move in the strongly strained and corrugated "laminar" mixing layers. See Peters and Williams (1983) for an attempt to evaluate the lift-off height using percolation ideas. The flame spread is not possible in regions where a large enough fraction of the corrugated laminar mixing layers can not sustain a diffusion flame, because they are subject to excessive strain.

5. DIFFUSION FLAMES IN STRAINED MIXING LAYERS

In turbulent flows the thin mixing layers between the fuel and air are distorted and strained by the flow field. A positive strain leads to a growth of the area covered by the fluid particles in the mixing layer and enhances the mixing process. The strain rate A is the inverse of a time that replaces the residence time a/U in the definition of the Damköhler number. For the diffusion flame to exist the strain rate can not exceed a critical extinction value A_E.

We shall give below a short description of the ignition and extinction processes in strained diffusions flames. A detailed account of ignition and extinction in diffusion flames may be found in Williams (1985); for applications of these ideas to turbulent diffusion flames, see Peters (1986).

For simplicity in the presentation, we shall use the thermal diffusive approximation in the description of the velocity field. We shall describe a planar mixing layer between two counter-flowing, two-dimensional, streams of fuel and oxidizer. The velocity field that we consider is the potential field, given by

$$u = 0 \ , \quad v = -Ay \ , \quad w = Az \tag{58}$$

with a constant strain rate A.

The conservation equations for the temperature and mass fractions of the fuel and oxygen have similarity solutions with T, Y_F, Y_0 functions of the time t, the coordinate y, transverse to the mixing layer and the coordinate x in the direction perpendicular to the strain. If, for simplicity, we limit our discussion to the case of unit Lewis numbers with a constant thermal diffusivity, the conservation equations take the form

$$L(\alpha) = W_F/\rho \tag{59}$$

with

$$L(\alpha) = \frac{\partial \alpha}{\partial t} - Ay\frac{\partial \alpha}{\partial y} - D_T\frac{\partial^2 \alpha}{\partial y^2} - D_T\frac{\partial^2 \alpha}{\partial x^2} \tag{60}$$

$\alpha = \{Y_F, Y_0/\nu_0,\ c_pT/q\}$ and

$$W_F/\rho = -Be^{-E/RT}Y_0Y_F \tag{61}$$

to be solved with the boundary conditions

$$y \to \infty : T - T_0 = Y_0 - Y_{00} = Y_F = 0 \tag{62a}$$

$$y \to -\infty : T - T_0 = Y_0 = Y_F - Y_{FO} = 0 \tag{62b}$$

and initial conditions

$$t = 0 : T = T_I(y,x)\ ,\ Y_F = Y_{FI}(y,x)\ ,\ Y_0 = Y_{OI}(y,x)\ . \tag{63}$$

It is easy to show that, independently of the initial conditions the mixture fraction variable Z and the excess temperature H, defined by Eqs. (22) and (30), which satisfy the boundary conditions $Z = H = 0$ at $y \to \infty$ and $Z - 1 = H = 0$ at $y \to -\infty$, are given for large times by

$$H = 0\ ,\ Z = \frac{1}{2}erfc(y/\sqrt{2D_T/A})\ . \tag{64}$$

We shall, for simplicity, consider that the initial concentrations and temperature are such that (64) also holds at $t = 0$.

The system of equations (61)-(64) can thus be reduced to the solution of the following equation

$$\frac{\partial \theta}{\partial t} - y\frac{\partial \theta}{\partial y} - \frac{\partial^2 \theta}{\partial y^2} - \frac{\partial^2 \theta}{\partial x^2} = D_0\hat{Y}_F\hat{Y}_0e^{\beta_0\theta/(1+\alpha_0\theta)} \tag{65}$$

for $\theta = c_p(T - T_0)/qY_{FO}$ in terms of the coordinates x, y and time t, scaled here with the thickness $\delta_m = \sqrt{D_T/A}$ of the mixing layer and the time A^{-1}.

Here the D_0 is a Damköhler number

$$D_0 = A^{-1}BY_{00}\exp(-E/RT_0) \tag{66}$$

and

$$\alpha_0 = qY_{FO}/c_pT_0\ ,\ \beta_0 = (E/RT_0)(qY_{FO}/c_pT_0)\ . \tag{67}$$

Eq. (66) has to be solved with the boundary conditions

$$\theta = 0 \quad \text{for} \quad y \to \pm\infty\ . \tag{68}$$

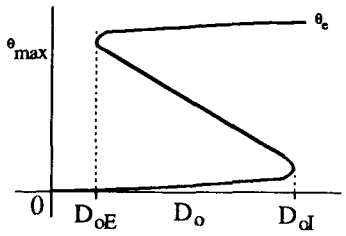

Figure 3. The maximum temperature in the mixing layer as a function of the Damköhler number.

The reduced mass fractions $\hat{Y}_F$ and $\hat{Y}_0$ are given by the relations

$$\hat{Y}_F + \theta = 1 - \hat{Y}_0 - S\theta = Z = \frac{1}{2} erfc(y/\sqrt{2}) \; . \tag{69}$$

We should add an initial condition

$$t = 0 : \quad \theta = \theta_I(y, x) \; . \tag{70}$$

5.1 One dimensional steady solutions

There are one dimensional steady solutions of this problem, in the form $\theta = \theta(y)$ given by the equation

$$y\frac{\partial \theta}{\partial y} + \frac{\partial^2 \theta}{\partial y^2} = -D_a \hat{Y}_F \hat{Y}_0 e^{\beta_0 \theta/(1+\alpha_0 \theta)} \tag{71}$$

with $\theta = 0$ at $y \to \pm\infty$.

This problem has multiple solutions for values of the Zeldovich number β_0, larger than a critical value $\beta_c(\alpha_0, S)$. These are sketched in Fig. 3.

Liñán (1974) has carried our an asymptotic description of the solution of Eq. (71), for large values of the Zeldovich number, to calculate the ignition and extinction conditions, and the interval (D_{OE}, D_{OI}) of multiplicity of solutions.

We simply indicate here that for large Damköhler numbers, the maximum temperature in the nearly frozen solution for $D_0 < D_{OI}$ differs from O only by an amount of order $1/\beta_0$

at most. In the upper, diffusion controlled solution, for $D_0 > D_{OE}$, $\theta_{\max}$ is close to the adiabatic flame temperature θ_e corresponding to the $(B-S)$ solution of infinite Damköhler numbers. In this $(B-S)$ limit:

$$\hat{Y}_0 = 0 \quad \text{for} \quad Z > Z_s \,, \; \hat{Y}_F = 0 \quad \text{for} \quad Z < Z_s \tag{72}$$

and the flame sheet is located at $y = y_f$, given by

$$Z_s = \frac{1}{2} erfc(y_f/\sqrt{2}) \,, \tag{73}$$

and there the flame temperature takes the value $\theta_e = Z_s = 1/(S+1)$.

The intermediate, unstable, branch has reaction sheet temperatures θ_f, given approximately, by the following balance

$$1 = D_0 \exp\{\beta_0 \theta_f/(1+\alpha_0\theta_f)\} \tag{74}$$

obtained from a rough order of magnitude estimate of the terms in Eq. (71), leaving aside a power factor of β_0.

When D_0 is such that the temperature θ_f given by (74) equals 0, the resulting value of $D_{OE} = 1$ is a rough estimate of D_{OI}. Similarly the Damköhler number given by Eq. (74) with $\theta_f = \theta_e$ is a rough estimate of the extinction value of D_0.

5.2 Ignition and Extinction Fronts

In the Damköhler number interval between the extinction and ignition values, the nearly frozen solutions and the near equilibrium solutions may coexist in the mixing layer; we could encounter the first one at large negative values of x, and the near-equilibrium solution at large positive values of x, joined by a transition front as shown in Fig. 4.

Eq. (65) has travelling wave solutions of the form $\theta = \theta(x', y)$, with $x' = x + U_p t$, joining the two solutions. They are given by the equation

$$U_F \theta_{x'} - y\theta_y - \theta_{yy} - \theta_{x'x'} = D_0 \hat{Y}_F \hat{Y}_0 \exp\{\beta_0\theta/(1+\alpha_0\theta)\} \tag{75}$$

to be solved with the boundary conditions

$$\theta = 0 \quad \text{for} \quad y \to \pm\infty \tag{76}$$

and

$$\theta = \theta_l(y) \quad \text{for} \quad x' \to -\infty \tag{77}$$

$$\theta = \theta_u(y) \quad \text{for} \quad x' \to \infty \tag{78}$$

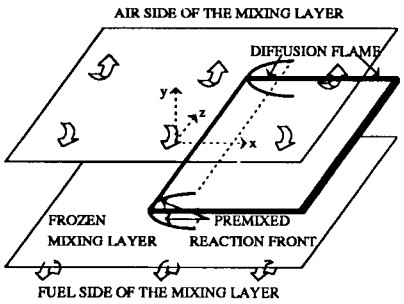

Figure 4. Schematic description of an ignition or extinction front in a strained mixing layer.

where θ_l and θ_u are the lower (nearly frozen) and upper (near-equilibrium) solution of Eq. (71). U_F is the velocity of propagation of the front, an eigenvalue of the problem,

$$U_F = U_F(D_0, \beta_0, \alpha_0, S) \; . \tag{79}$$

The resulting value of U_F is positive for ignition fronts, for values of $D_0 > D_0^c$, and U will be negative for values of $D_0 < D_0^c$, corresponding to extinction fronts.

A considerable effort is being currently devoted to the analysis of ignition and extinction fronts; see, for example, the initial work of Dold (1987) and Liñán (1988). These fronts may play an important role in the lift-off and blow-off characteristics of turbulent diffusion flames. The thermal expansion effects, left out in the analysis of these fronts given here, will significantly alter their propagation velocity.

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